

Curriculum Vitae

PERSONAL INFORMATION

Family name, First name: Grajciar, Lukáš

Researcher unique identifier(s): [0000-0001-9464-7769](https://orcid.org/0000-0001-9464-7769) (ORCID), [H-1266-2015](https://publons.com/urn/hid:publons:H-1266-2015) (Researcher ID)

Date of birth: 05.02.1985

Nationality: Slovak

URL for web site: <http://physchem.cz/people/dr-lukas-grajciar/>

PUBLICATIONS

- **33 papers** in SCI journals included in ISI Core Collection
- **2 as single** author and additional **7 as first** author, **6 as senior corresponding** author
- **1428 citations** without self-citations, h-index = **18**

• CURRENT POSITION

2020 – Assistant Professor
Faculty of Science, Charles University, Czech Republic
Junior group leader research project (**two postdocs and one PhD student**), Charles University ([Primus/20/SCI/004](https://primus.cuni.cz/20/SCI/004)): Computational catalysis goes operando

• PREVIOUS POSITIONS

2017 – 2020 Researcher
Faculty of Science, Charles University, Czech Republic
Member of the Charles University Centre of Advanced Materials (CUCAM - <http://cucam.cuni.cz>)

2015 – 2016 Independent researcher
University of Jena, Germany
Funded by self-acquired Deutsche Forschungsgemeinschaft (DFG) Grant No. 269386423
<http://gepris.dfg.de/gepris/projekt/269386423>

2013 – 2014 Postdoctoral researcher & Software developer
TURBOMOLE GmbH, Germany (<http://www.turbomole-gmbh.com>) & University of Jena, Germany
Funded by internal TURBOMOLE projects

• CURRENT RESEARCH INTERESTS

- Machine learning methods in chemistry (neural network-based potentials, machine learned collective variables, etc.), global optimizations for structure predictions, free energy methods, density functional theory calculations
- Zeolite chemistry, dynamical treatment of liquid-solid interface, heterogenous catalysis in microporous materials (zeolites, MOFs)

• EDUCATION

2009-2013 PhD in study field: Modelling of chemical properties of nano- and biostructures
Faculty of Science, Charles University, Czech Republic
Supervisor: Petr Nachtigall
PhD Thesis: Theoretical investigation of chemical and physical properties of molecular sieves

2011 RNDr. in study field: Modelling of chemical properties of nano- and biostructures

Faculty of Science, Charles University, Czech Republic

2007-2009 MSc. in study field: Modelling of chemical properties of nano- and biostructures
Faculty of Science, Charles University, Czech Republic

- **SUPERVISION**

2017 – 3 PhD students as supervisor (**two defended**) and 4 PhD students as consultant (**three defended already**) at *Faculty of Science, Charles University, Czech Republic*
2018 – 2020 1 Master Student as supervisor (**defended**) at *Faculty of Science, Charles University, Czech Republic*
2017 – 2 Bachelor students as supervisor and 3 Bachelor students as consultant (**all three defended already**) at *Faculty of Science, Charles University, Czech Republic*

- **TEACHING ACTIVITIES**

2022 – **Lecturer** - “Quantum chemistry applications - materials properties and materials design” course at *Charles University, Czech Republic*; **course guarantor**, (33% share in teaching)
2017 – **Lecturer** - “Quantum Chemistry” course at *Charles University, Czech Republic*; **course guarantor since 2020**, (40% share in teaching)
2017 – **Lecturer** - “Electronic Structure of Complex Molecular Systems and Biomolecules” course at *Charles University, Czech Republic*; co-lectured (40% share in teaching)
2010 – 2013 **Undergraduate demonstrator**, *Charles University, Czech Republic*

- **SHORT RESEARCH STAYS**

07/2011 **Visiting researcher**, *University of Pittsburgh, USA* (with Prof. K. D. Jordan)
(2 weeks)
04/2011 **Visiting researcher**, *University of Edinburgh, UK* (with Prof. T. Düren)
(1 week)
07-09/2008 **Research student**, *Humboldt University, Berlin, Germany* (with Prof. J. Sauer)
(3 months)

- **AWARDS**

2014 **Prize of the Ministry of Education, Youth and Sports of the Czech Republic for outstanding academic achievement in postgraduate study program (2014)**, awarded each year to 3-4 laureates across all the postdoctoral study programs in Czech Republic (link - [Czech only](#))
2013 **Prize of the Dean of the Faculty of Science for an outstanding doctorate thesis (2013)**, single in chemistry postdoctoral study programs (link - [Czech only](#))